

STRUCTURE AND FUNCTIONS OF WATER-MEMBRANE INTERFACES AND THEIR ROLE IN PROTO-BIOLOGICAL EVOLUTION

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Among the most important developments in proto-biological evolution was the emergence of membrane-like structures. These are formed by spontaneous association of relatively simple amphiphilic molecules that would have been readily available in the primordial environment. The resulting interfacial regions between water and nonpolar interior of the membrane have several properties which made them uniquely suitable for promoting subsequent evolution. They can a) selectively attract organic material and mediate its transport, b) serve as simple catalysts for chemical reactions, and c) promote the formation of trans-membrane electrical and chemical gradients which could provide energy sources for proto-cells. Understanding the structure of interfaces, their interactions with organic molecules and molecular mechanisms of their functions is an essential step to understanding proto-biological evolution.

In our computer simulation studies, we showed that the structure of water at interfaces with nonpolar media is significantly different from that in the bulk. In particular, the average surface dipole density points from the vapor to the liquid. As a result, negative ions can approach the interface more easily than positive ions. Amphiphilic molecules composed of hydrocarbon conjugated rings and polar substituents (e.g., phenol) assume at the interface rigid orientations in which polar groups are buried in water while hydrocarbon parts are located in the nonpolar environment. These orientational differences are of special interest in connection with the ability of some of these molecules to efficiently absorb photons. Flexible molecules with polar substituents often adopt at interfaces conformations different from those in the bulk aqueous solution and in the gas phase. As a result, in many instances both specificity and kinetics of chemical reactions in which these molecules can participate is modified by the presence of surfaces.

Of special interest is the mechanism by which polar molecules are transferred across interface between water and a nonpolar medium. Our recent study showed that simple ionophores bind ions by the same mechanisms as ion channels and carriers from modern cells. In particular, upon binding the ion these ionophores undergo change in which their polar groups come into close contact with the ion and get buried in the interior of the carrier. Simultaneously, groups soluble in oil become exposed to the surface allowing the complex to penetrate the oily environment of the membrane. Thus, our study lends support to one of the main concepts in studies of biochemical evolution: that physico-chemical mechanisms of ubiquitous cell functions remained similar throughout evolution, but became more accurate and efficient as the molecules performing these functions gained structural complexity.